ELSEVIER

Chemical Physics 219 (1997) 359–362

Chemical Physics

Author index to volume 219

Abraham, E., J. Oberlé, G. Jonusauskas, R. Lapouyade, K. Minoshima and C. Rullière, Picosecond time-resolved dual fluorescence, transient absorption and reorientation time measurements of push–pull diphenyl-polyenes: evidence for 'loose' complex and 'bicimer' species 219 (1997) 73

Ahmed, M., C.J. Apps, M.J. Bramwell, J.L. Cooper, C. Hughes, K. Reinhardt, J.C. Whitehead, F. Winterbottom and A. Hopkirk, Fluorescence excitation spectroscopy of some haloethenes, $CF_2=CXY$ (XY ≡ FCl, Cl_2, FH), excited in the vacuum ultraviolet (70–180 nm) 219 (1997) 333

Aloisio, S. and J.S. Francisco, Ab initio study of the structure, vibrational spectra and binding energy of HCl–ClO and Cl_2–ClO complexes 119 (1997) 201

Apkarian, V.A., see Grigorenko, B.L. 219 (1997) 161

Apps, C.J., see Ahmed, M. 219 (1997) 333

Asawakun, P., see Sagarik, K. 219 (1997) 173

Baltzer, P., see Holland, D.M.P. 219 (1997) 91

Baraille, I., see Habas, M.-P. 219 (1997) 63

Beckmann, S., see Steybe, F. 219 (1997) 317

Benderskii, V.A., E.V. Vetoshkin, L. von Laue and H.P. Trommsdorff, Tunneling splitting in vibrational spectra of non-rigid molecules. II. Excited states 219 (1997) 143

Benderskii, V.A., E.V. Vetoshkin, S.Yu. Grebenshchikov, L. von Laue and H.P. Trommsdorff, Tunneling splitting in vibrational spectra of non-rigid molecules. I. Perturbative instanton approach 219 (1997) 119

Boldyrev, S.I., see Coropceanu, V.P. 219 (1997) 1

Bouteiller, Y., see Coussan, S. 219 (1997) 221

Bramwell, M.J., see Ahmed, M. 219 (1997) 333

Carrington Jr., T., see Krishnan, M.S. 219 (1997) 31

Chaillet, M., see Habas, M.-P. 219 (1997) 63

Cooper, J.L., see Ahmed, M. 219 (1997) 333

Coropceanu, V.P., F.G. Paladi, S.I. Boldyrev and V.J. Gamurar, Double exchange in tetrameric tetrahedral clusters with two-electron transfer: magnetic properties 219 (1997) 1

Cortés, J. and E. Valencia, Commensurability and transformations of adsorbed phases on a heterogeneous solid with periodic distribution of surface energy 219 (1997) 235

Coussan, S., Y. Bouteiller, A. Loutellier, J.P. Perchard, S. Racine, A. Peremans, W.Q. Zheng and A. Tadjeddine, Infrared photoisomerization of the methanol dimer trapped in argon matrix: monochromatic irradiation experiments and DFT calculations 219 (1997) 221

De Lara-Castells, M.P., see Gianturco, F.A. 219 (1997) 117

Delysse, S., P. Raimond and J.-M. Nunzi, Two-photon absorption in non-centrosymmetric dyes 219 (1997) 341

Effenberger, F., see Steybe, F. 219 (1997) 317

Francisco, J.S., see Aloisio, S. 119 (1997) 201

Gamurar, V.J., see Coropceanu, V.P. 219 (1997) 1
Germain, A. and P. Millié, Localization of σ molecular orbitals: towards a better description of the electronic excited states of large conjugated molecules 219 (1997) 265
Gianturco, F.A. and M.P. de Lara-Castells, Structure and anisotropy of ionic argon clusters using density functional models [Chem. Phys. 208 (1996) 25–34]. Erratum 219 (1997) 117
Glania, C., see Steybe, F. 219 (1997) 317
Granucci, G., see Romstad, D. 219 (1997) 21
Grebenshchikov, S.Yu., see Benderskii, V.A. 219 (1997) 119
Grigorenko, B.L., A.V. Nemukhin and V.A. Apkarian, Inclusion of ion-pair states in the diatomics-in-molecules description of potential energy surfaces: van der Waals complexes of $He–Cl_2$ and $Ar–Cl_2$ 219 (1997) 161

Habas, M.-P., I. Baraille, C. Larrieu and M. Chaillet, Ab initio calculation of the electronic spectrum and ionization potentials of hydrazine 219 (1997) 63
Hannongbua, S., see Tongraar, A. 219 (1997) 279
Hayes, M.A., see Holland, D.M.P. 219 (1997) 91
Holland, D.M.P., D.A. Shaw, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, L. Karlsson, P. Baltzer and B. Wannberg, A photoabsorption, photodissociation and photoelectron spectroscopy study of C_2H_4 and C_2D_4 219 (1997) 91
Hopkirk, A., see Ahmed, M. 219 (1997) 333
Hughes, C., see Ahmed, M. 219 (1997) 333

Iwata, S., see Li, Y. 219 (1997) 209

Jonusauskas, G., see Abraham, E. 219 (1997) 73
Jursic, B.S., Hybrid density functional theory, Gaussian, and complete basis set ab initio studies of the stability of aluminum monocarbonyl and aluminum isocarbonyl 219 (1997) 57

Kalotas, T.M., see Mellor, W.E. 219 (1997) 257
Karlsson, L., see Holland, D.M.P. 219 (1997) 91
Knüpling, M., J.T. Törring and S. Un, The relationship between the molecular structure of semiquinone radicals and their *g*-values 219 (1997) 291
Kosterev, A.A., A.A. Makarov, A.L. Malinovsky and E.A. Ryabov, Fast collision-induced redistribution of vibrational energy in halogenated methanes 219 (1997) 305
Krämer, P., see Steybe, F. 219 (1997) 317
Krishnan, M.S. and T. Carrington Jr., Uncoupled effective Hamiltonians for molecules with several vibrational modes coupled by Coriolis and centrifugal terms 219 (1997) 31

Lapouyade, R., see Abraham, E. 219 (1997) 73
Larrieu, C., see Habas, M.-P. 219 (1997) 63
Lee, A.R., see Mellor, W.E. 219 (1997) 257
Lee, S.-L., see Slanina, Z. 219 (1997) 193
Li, Y. and S. Iwata, Theoretical study of cyclic radicals NO_x ($x = 2–6$) 219 (1997) 209

Lifshitz, A. and H. Teitelbaum, The unusual effect of reagent vibrational excitation on the rates of endothermic and exothermic elementary combustion reactions 219 (1997) 243
Loutellier, A., see Coussan, S. 219 (1997) 221

Makarov, A.A., see Kosterev, A.A. 219 (1997) 305
Malinovsky, A.L., see Kosterev, A.A. 219 (1997) 305
Mellor, W.E., A.R. Lee and T.M. Kalotas, Alternative calculations for internal rotations: Assessment via Mathieu and multi-Fourier term potentials 219 (1997) 257
Millié, P., see Germain, A. 219 (1997) 265
Minoshima, K., see Abraham, E. 219 (1997) 73

Nemukhin, A.V., see Grigorenko, B.L. 219 (1997) 161
Nunzi, J.-M., see Delysse, S. 219 (1997) 341

Oberlé, J., see Abraham, E. 219 (1997) 73
Ōsawa, E., see Slanina, Z. 219 (1997) 193

Paladi, F.G., see Coropceanu, V.P. 219 (1997) 1
Perchard, J.P., see Coussan, S. 219 (1997) 221
Peremans, A., see Coussan, S. 219 (1997) 221
Persico, M., see Romstad, D. 219 (1997) 21
Pesce, L. and P. Saalfrank, "Free" nuclear density propagation in two dimensions. The coupled-channel density matrix method and its application to inelastic molecule–surface scattering 219 (1997) 43

Racine, S., see Coussan, S. 219 (1997) 221
Raimond, P., see Delysse, S. 219 (1997) 341
Reinhardt, K., see Ahmed, M. 219 (1997) 333
Rennie, E.E., see Holland, D.M.P. 219 (1997) 91
Rode, B.M., see Tongraar, A. 219 (1997) 279
Romstad, D., G. Granucci and M. Persico, Nonadiabatic transitions and interference in photodissociation dynamics 219 (1997) 21
Rullière, C., see Abraham, E. 219 (1997) 73
Ryabov, E.A., see Kosterev, A.A. 219 (1997) 305

Saalfrank, P., see Pesce, L. 219 (1997) 43
Sagarik, K. and P. Asawakun, Intermolecular potential for phenol based on the test particle model 219 (1997) 173
Shaw, D.A., see Holland, D.M.P. 219 (1997) 91
Shpinkova, L.G., see Holland, D.M.P. 219 (1997) 91
Slanina, Z., X. Zhao, S.-L. Lee and E. Ōsawa, C_{90} temperature effects on relative stabilities of the IPR isomers 219 (1997) 193
Steybe, F., F. Effenberger, S. Beckmann, P. Krämer, C. Glania and R. Wortmann, Enhanced nonlinear optical properties and thermal stability of donor–acceptor substituted oligothiophenes 219 (1997) 317

Tadjeddine, A., see Coussan, S. 219 (1997) 221
Teitelbaum, H., see Lifshitz, A. 219 (1997) 243

Tongraar, A., S. Hannongbua and B.M. Rode, Molecular dynamics simulations of a potassium ion and an iodide ion in liquid ammonia 219 (1997) 279
Törring, J.T., see Knüpling, M. 219 (1997) 291
Trommsdorff, H.P., see Benderskii, V.A. 219 (1997) 119
Trommsdorff, H.P., see Benderskii, V.A. 219 (1997) 143

Un, S., see Knüpling, M. 219 (1997) 291

Valencia, E., see Cortés, J. 219 (1997) 235
Vetoshkin, E.V., see Benderskii, V.A. 219 (1997) 119
Vetoshkin, E.V., see Benderskii, V.A. 219 (1997) 143
Von Laue, L., see Benderskii, V.A. 219 (1997) 119
Von Laue, L., see Benderskii, V.A. 219 (1997) 143

Wannberg, B., see Holland, D.M.P. 219 (1997) 91
Whitehead, J.C., see Ahmed, M. 219 (1997) 333
Winterbottom, F., see Ahmed, M. 219 (1997) 333
Wortmann, R., see Steybe, F. 219 (1997) 317

Zhang, Y., Photoacoustic spectra of BaFBr:Eu^{2+} phosphors 219 (1997) 353
Zhao, X., see Slanina, Z. 219 (1997) 193
Zheng, W.Q., see Coussan, S. 219 (1997) 221

ELSEVIER

Chemical Physics 219 (1997) 363–370

Chemical Physics

Subject index to volume 219

Methods

Theoretical

Group theory and algebras

Double exchange in tetrameric tetrahedral clusters with two-electron transfer: magnetic properties, V.P. Coropceanu, F.G. Paladi, S.I. Boldyrev and V.J. Gamurar 219 (1997) 1

Many body and quasiparticle approaches

Double exchange in tetrameric tetrahedral clusters with two-electron transfer: magnetic properties, V.P. Coropceanu, F.G. Paladi, S.I. Boldyrev and V.J. Gamurar 219 (1997) 1

Coupling schemes and perturbative treatments

Double exchange in tetrameric tetrahedral clusters with two-electron transfer: magnetic properties, V.P. Coropceanu, F.G. Paladi, S.I. Boldyrev and V.J. Gamurar 219 (1997) 1

Nonadiabatic transitions and interference in photodissociation dynamics, D. Romstad, G. Granucci and M. Persico 219 (1997) 21

Uncoupled effective Hamiltonians for molecules with several vibrational modes coupled by Coriolis and centrifugal terms, M.S. Krishnan and T. Carrington Jr. 219 (1997) 31

"Free" nuclear density propagation in two dimensions. The coupled-channel density matrix method and its application to inelastic molecule–surface scattering, L. Pesce and P. Saalfrank 219 (1997) 43

Tunneling splitting in vibrational spectra of non-rigid molecules. I. Perturbative instanton approach, V.A. Benderskii, E.V. Vetoshkin, S.Yu. Grebenshchikov, L. von Laue and H.P. Trommsdorff 219 (1997) 119

Tunneling splitting in vibrational spectra of non-rigid molecules. II. Excited states, V.A. Benderskii, E.V. Vetoshkin, L. von Laue and H.P. Trommsdorff 219 (1997) 143

Inclusion of ion-pair states in the diatomics-in-molecules description of potential energy surfaces: van der Waals complexes of $He–Cl_2$ and $Ar–Cl_2$, B.L. Grigorenko, A.V. Nemukhin and V.A. Apkarian 219 (1997) 161

Equilibrium statistical mechanics

Intermolecular potential for phenol based on the test particle model, K. Sagarik and P. Asawakun 219 (1997) 173

C_{90} temperature effects on relative stabilities of the IPR isomers, Z. Slanina, X. Zhao, S.-L. Lee and E. Ōsawa 219 (1997) 193

Ab initio schemes for stationary properties
Ab initio study of the structure, vibrational spectra and binding energy of HCl–ClO and Cl_2–ClO complexes, S. Aloisio and J.S. Francisco 119 (1997) 201
Hybrid density functional theory, Gaussian, and complete basis set ab initio studies of the stability of aluminum monocarbonyl and aluminum isocarbonyl, B.S. Jursic 219 (1997) 57
Ab initio calculation of the electronic spectrum and ionization potentials of hydrazine, M.-P. Habas, I. Baraille, C. Larrieu and M. Chaillet 219 (1997) 63
Intermolecular potential for phenol based on the test particle model, K. Sagarik and P. Asawakun 219 (1997) 173
C_{90} temperature effects on relative stabilities of the IPR isomers, Z. Slanina, X. Zhao, S.-L. Lee and E. Ōsawa 219 (1997) 193
Theoretical study of cyclic radicals NO_x ($x = 2$–6), Y. Li and S. Iwata 219 (1997) 209
Infrared photoisomerization of the methanol dimer trapped in argon matrix: monochromatic irradiation experiments and DFT calculations, S. Coussan, Y. Bouteiller, A. Loutellier, J.P. Perchard, S. Racine, A. Peremans, W.Q. Zheng and A. Tadjeddine 219 (1997) 221

Computational and simulation methods
Uncoupled effective Hamiltonians for molecules with several vibrational modes coupled by Coriolis and centrifugal terms, M.S. Krishnan and T. Carrington Jr. 219 (1997) 31
C_{90} temperature effects on relative stabilities of the IPR isomers, Z. Slanina, X. Zhao, S.-L. Lee and E. Ōsawa 219 (1997) 193
Commensurability and transformations of adsorbed phases on a heterogeneous solid with periodic distribution of surface energy, J. Cortés and E. Valencia 219 (1997) 235
The unusual effect of reagent vibrational excitation on the rates of endothermic and exothermic elementary combustion reactions, A. Lifshitz and H. Teitelbaum 219 (1997) 243
Alternative calculations for internal rotations: Assessment via Mathieu and multi-Fourier term potentials, W.E. Mellor, A.R. Lee and T.M. Kalotas 219 (1997) 257
Localization of σ molecular orbitals: towards a better description of the electronic excited states of large conjugated molecules, A. Germain and P. Millié 219 (1997) 265

Molecular dynamics and scattering theory
"Free" nuclear density propagation in two dimensions. The coupled-channel density matrix method and its application to inelastic molecule–surface scattering, L. Pesce and P. Saalfrank 219 (1997) 43
Molecular dynamics simulations of a potassium ion and an iodide ion in liquid ammonia, A. Tongraar, S. Hannongbua and B.M. Rode 219 (1997) 279
The relationship between the molecular structure of semiquinone radicals and their *g*-values, M. Knüpling, J.T. Törring and S. Un 219 (1997) 291

Experimental

Infrared spectroscopy
Infrared photoisomerization of the methanol dimer trapped in argon matrix: monochromatic irradiation experiments and DFT calculations, S. Coussan, Y. Bouteiller, A. Loutellier, J.P. Perchard, S. Racine, A. Peremans, W.Q. Zheng and A. Tadjeddine 219 (1997) 221

Raman spectroscopy
Fast collision-induced redistribution of vibrational energy in halogenated methanes, A.A. Kosterev, A.A. Makarov, A.L. Malinovsky and E.A. Ryabov 219 (1997) 305

Visible and UV spectroscopy
Ab initio calculation of the electronic spectrum and ionization potentials of hydrazine, M.-P. Habas, I. Baraille, C. Larrieu and M. Chaillet 219 (1997) 63
Localization of σ molecular orbitals: towards a better description of the electronic excited states of large conjugated molecules, A. Germain and P. Millié 219 (1997) 265
Enhanced nonlinear optical properties and thermal stability of donor–acceptor substituted oligothiophenes, F. Steybe, F. Effenberger, S. Beckmann, P. Krämer, C. Glania and R. Wortmann 219 (1997) 317
Fluorescence excitation spectroscopy of some haloethenes, $CF_2=CXY$ (XY ≡ FCl, Cl_2, FH), excited in the vacuum ultraviolet (70–180 nm), M. Ahmed, C.J. Apps, M.J. Bramwell, J.L. Cooper, C. Hughes, K. Reinhardt, J.C. Whitehead, F. Winterbottom and A. Hopkirk 219 (1997) 333

Fluorescence spectroscopy
Picosecond time-resolved dual fluorescence, transient absorption and reorientation time measurements of push–pull diphenyl-polyenes: evidence for 'loose' complex and 'bicimer' species, E. Abraham, J. Oberlé, G. Jonusauskas, R. Lapouyade, K. Minoshima and C. Rullière 219 (1997) 73
Localization of σ molecular orbitals: towards a better description of the electronic excited states of large conjugated molecules, A. Germain and P. Millié 219 (1997) 265
Fluorescence excitation spectroscopy of some haloethenes, $CF_2=CXY$ (XY ≡ FCl, Cl_2, FH), excited in the vacuum ultraviolet (70–180 nm), M. Ahmed, C.J. Apps, M.J. Bramwell, J.L. Cooper, C. Hughes, K. Reinhardt, J.C. Whitehead, F. Winterbottom and A. Hopkirk 219 (1997) 333

Photoelectron and Auger spectroscopy
A photoabsorption, photodissociation and photoelectron spectroscopy study of C_2H_4 and C_2D_4, D.M.P. Holland, D.A. Shaw, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, L. Karlsson, P. Baltzer and B. Wannberg 219 (1997) 91

Laser methods
Infrared photoisomerization of the methanol dimer trapped in argon matrix: monochromatic irradiation experiments and DFT calculations, S. Coussan, Y. Bouteiller, A. Loutellier, J.P. Perchard, S. Racine, A. Peremans, W.Q. Zheng and A. Tadjeddine 219 (1997) 221

Picosecond spectroscopy
Two-photon absorption in non-centrosymmetric dyes, S. Delysse, P. Raimond and J.-M. Nunzi 219 (1997) 341

Non-linear optical spectroscopy
Two-photon absorption in non-centrosymmetric dyes, S. Delysse, P. Raimond and J.-M. Nunzi 219 (1997) 341

Synchrotron spectroscopies
A photoabsorption, photodissociation and photoelectron spectroscopy study of C_2H_4 and C_2D_4, D.M.P. Holland, D.A. Shaw, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, L. Karlsson, P. Baltzer and B. Wannberg 219 (1997) 91

Fluorescence excitation spectroscopy of some haloethenes, $CF_2=CXY$ (XY ≡ FCl, Cl_2, FH), excited in the vacuum ultraviolet (70–180 nm), M. Ahmed, C.J. Apps, M.J. Bramwell, J.L. Cooper, C. Hughes, K. Reinhardt, J.C. Whitehead, F. Winterbottom and A. Hopkirk 219 (1997) 333

Optical pumping
Photoacoustic spectra of $BaFBr:Eu^{2+}$ phosphors, Y. Zhang 219 (1997) 353

Atomic and molecular beam techniques
Fluorescence excitation spectroscopy of some haloethenes, $CF_2=CXY$ (XY ≡ FCl, Cl_2, FH), excited in the vacuum ultraviolet (70–180 nm), M. Ahmed, C.J. Apps, M.J. Bramwell, J.L. Cooper, C. Hughes, K. Reinhardt, J.C. Whitehead, F. Winterbottom and A. Hopkirk 219 (1997) 333

Time-resolved experiments
Picosecond time-resolved dual fluorescence, transient absorption and reorientation time measurements of push–pull diphenyl-polyenes: evidence for 'loose' complex and 'bicimer' species, E. Abraham, J. Oberlé, G. Jonusauskas, R. Lapouyade, K. Minoshima and C. Rullière 219 (1997) 73

Objects

Bulk systems

Liquid mixtures and solutions
Intermolecular potential for phenol based on the test particle model, K. Sagarik and P. Asawakun 219 (1997) 173

Semiconductors
Photoacoustic spectra of $BaFBr:Eu^{2+}$ phosphors, Y. Zhang 219 (1997) 353

Surfaces
Commensurability and transformations of adsorbed phases on a heterogeneous solid with periodic distribution of surface energy, J. Cortés and E. Valencia 219 (1997) 235

Microscopic systems

Atoms
The unusual effect of reagent vibrational excitation on the rates of endothermic and exothermic elementary combustion reactions, A. Lifshitz and H. Teitelbaum 219 (1997) 243
Molecular dynamics simulations of a potassium ion and an iodide ion in liquid ammonia, A. Tongraar, S. Hannongbua and B.M. Rode 219 (1997) 279

Molecules (neutral and ionic)
Tunneling splitting in vibrational spectra of non-rigid molecules. I. Perturbative instanton approach, V.A. Benderskii, E.V. Vetoshkin, S.Yu. Grebenshchikov, L. von Laue and H.P. Trommsdorff 219 (1997) 119

Tunneling splitting in vibrational spectra of non-rigid molecules. II. Excited states, V.A. Benderskii, E.V. Vetoshkin, L. von Laue and H.P. Trommsdorff 219 (1997) 143
Alternative calculations for internal rotations: Assessment via Mathieu and multi-Fourier term potentials, W.E. Mellor, A.R. Lee and T.M. Kalotas 219 (1997) 257

-diatomic
Nonadiabatic transitions and interference in photodissociation dynamics, D. Romstad, G. Granucci and M. Persico 219 (1997) 21
"Free" nuclear density propagation in two dimensions. The coupled-channel density matrix method and its application to inelastic molecule–surface scattering, L. Pesce and P. Saalfrank 219 (1997) 43
The unusual effect of reagent vibrational excitation on the rates of endothermic and exothermic elementary combustion reactions, A. Lifshitz and H. Teitelbaum 219 (1997) 243

-small polyatomics
Ab initio study of the structure, vibrational spectra and binding energy of HCl–ClO and Cl_2–ClO complexes, S. Aloisio and J.S. Francisco 119 (1997) 201
Uncoupled effective Hamiltonians for molecules with several vibrational modes coupled by Coriolis and centrifugal terms, M.S. Krishnan and T. Carrington Jr. 219 (1997) 31
Hybrid density functional theory, Gaussian, and complete basis set ab initio studies of the stability of aluminum monocarbonyl and aluminum isocarbonyl, B.S. Jursic 219 (1997) 57
Ab initio calculation of the electronic spectrum and ionization potentials of hydrazine, M.-P. Habas, I. Baraille, C. Larrieu and M. Chaillet 219 (1997) 63
A photoabsorption, photodissociation and photoelectron spectroscopy study of C_2H_4 and C_2D_4, D.M.P. Holland, D.A. Shaw, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, L. Karlsson, P. Baltzer and B. Wannberg 219 (1997) 91
Theoretical study of cyclic radicals NO_x ($x = 2$–6), Y. Li and S. Iwata 219 (1997) 209
Alternative calculations for internal rotations: Assessment via Mathieu and multi-Fourier term potentials, W.E. Mellor, A.R. Lee and T.M. Kalotas 219 (1997) 257
Fast collision-induced redistribution of vibrational energy in halogenated methanes, A.A. Kosterev, A.A. Makarov, A.L. Malinovsky and E.A. Ryabov 219 (1997) 305

-aromatics
Picosecond time-resolved dual fluorescence, transient absorption and reorientation time measurements of push–pull diphenyl-polyenes: evidence for 'loose' complex and 'bicimer' species, E. Abraham, J. Oberlé, G. Jonusauskas, R. Lapouyade, K. Minoshima and C. Rullière 219 (1997) 73
The relationship between the molecular structure of semiquinone radicals and their *g*-values, M. Knüpling, J.T. Törring and S. Un 219 (1997) 291

-other large
Enhanced nonlinear optical properties and thermal stability of donor–acceptor substituted oligothiophenes, F. Steybe, F. Effenberger, S. Beckmann, P. Krämer, C. Glania and R. Wortmann 219 (1997) 317
Two-photon absorption in non-centrosymmetric dyes, S. Delysse, P. Raimond and J.-M. Nunzi 219 (1997) 341

Molecular aggregates
Inclusion of ion-pair states in the diatomics-in-molecules description of potential energy surfaces: van der Waals complexes of He–Cl_2 and Ar–Cl_2, B.L. Grigorenko, A.V. Nemukhin and V.A. Apkarian 219 (1997) 161
Intermolecular potential for phenol based on the test particle model, K. Sagarik and P. Asawakun 219 (1997) 173

-dimers
Infrared photoisomerization of the methanol dimer trapped in argon matrix: monochromatic irradiation experiments and DFT calculations, S. Coussan, Y. Bouteiller, A. Loutellier, J.P. Perchard, S. Racine, A. Peremans, W.Q. Zheng and A. Tadjeddine 219 (1997) 221

-van der Waals molecules
Ab initio study of the structure, vibrational spectra and binding energy of HCl–ClO and Cl_2–ClO complexes, S. Aloisio and J.S. Francisco 119 (1997) 201
Inclusion of ion-pair states in the diatomics-in-molecules description of potential energy surfaces: van der Waals complexes of He–Cl_2 and Ar–Cl_2, B.L. Grigorenko, A.V. Nemukhin and V.A. Apkarian 219 (1997) 161

-clusters
Double exchange in tetrameric tetrahedral clusters with two-electron transfer: magnetic properties, V.P. Coropceanu, F.G. Paladi, S.I. Boldyrev and V.J. Gamurar 219 (1997) 1
C_{90} temperature effects on relative stabilities of the IPR isomers, Z. Slanina, X. Zhao, S.-L. Lee and E. Ōsawa 219 (1997) 193

-complexes
Hybrid density functional theory, Gaussian, and complete basis set ab initio studies of the stability of aluminum monocarbonyl and aluminum isocarbonyl, B.S. Jursic 219 (1997) 57
Molecular dynamics simulations of a potassium ion and an iodide ion in liquid ammonia, A. Tongraar, S. Hannongbua and B.M. Rode 219 (1997) 279

Free radicals (including hydronium and muonium)
Theoretical study of cyclic radicals NO_x ($x = 2$–6), Y. Li and S. Iwata 219 (1997) 209

Phenomena

Molecular structure
Ab initio study of the structure, vibrational spectra and binding energy of HCl–ClO and Cl_2–ClO complexes, S. Aloisio and J.S. Francisco 119 (1997) 201
Hybrid density functional theory, Gaussian, and complete basis set ab initio studies of the stability of aluminum monocarbonyl and aluminum isocarbonyl, B.S. Jursic 219 (1997) 57
C_{90} temperature effects on relative stabilities of the IPR isomers, Z. Slanina, X. Zhao, S.-L. Lee and E. Ōsawa 219 (1997) 193
Theoretical study of cyclic radicals NO_x ($x = 2$–6), Y. Li and S. Iwata 219 (1997) 209
The relationship between the molecular structure of semiquinone radicals and their *g*-values, M. Knüpling, J.T. Törring and S. Un 219 (1997) 291

Vibrations and rotations of molecules
Ab initio study of the structure, vibrational spectra and binding energy of HCl–ClO and Cl_2–ClO complexes, S. Aloisio and J.S. Francisco 119 (1997) 201
Uncoupled effective Hamiltonians for molecules with several vibrational modes coupled by Coriolis and centrifugal terms, M.S. Krishnan and T. Carrington Jr. 219 (1997) 31
Infrared photoisomerization of the methanol dimer trapped in argon matrix: monochromatic irradiation experiments and DFT calculations, S. Coussan, Y. Bouteiller, A. Loutellier, J.P. Perchard, S. Racine, A. Peremans, W.Q. Zheng and A. Tadjeddine 219 (1997) 221
Alternative calculations for internal rotations: Assessment via Mathieu and multi-Fourier term potentials, W.E. Mellor, A.R. Lee and T.M. Kalotas 219 (1997) 257
Fast collision-induced redistribution of vibrational energy in halogenated methanes, A.A. Kosterev, A.A. Makarov, A.L. Malinovsky and E.A. Ryabov 219 (1997) 305

Electronic structure and states
Nonadiabatic transitions and interference in photodissociation dynamics, D. Romstad, G. Granucci and M. Persico 219 (1997) 21
Ab initio calculation of the electronic spectrum and ionization potentials of hydrazine, M.-P. Habas, I. Baraille, C. Larrieu and M. Chaillet 219 (1997) 63
A photoabsorption, photodissociation and photoelectron spectroscopy study of C_2H_4 and C_2D_4, D.M.P. Holland, D.A. Shaw, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, L. Karlsson, P. Baltzer and B. Wannberg 219 (1997) 91
Theoretical study of cyclic radicals NO_x ($x = 2$–6), Y. Li and S. Iwata 219 (1997) 209
Localization of σ molecular orbitals: towards a better description of the electronic excited states of large conjugated molecules, A. Germain and P. Millié 219 (1997) 265
Fluorescence excitation spectroscopy of some haloethenes, CF_2=CXY (XY ≡ FCl, Cl_2, FH), excited in the vacuum ultraviolet (70–180 nm), M. Ahmed, C.J. Apps, M.J. Bramwell, J.L. Cooper, C. Hughes, K. Reinhardt, J.C. Whitehead, F. Winterbottom and A. Hopkirk 219 (1997) 333
Photoacoustic spectra of BaFBr:Eu^{2+} phosphors, Y. Zhang 219 (1997) 353
Two-photon absorption in non-centrosymmetric dyes, S. Delysse, P. Raimond and J.-M. Nunzi 219 (1997) 341

Molecular interactions
Intermolecular potential for phenol based on the test particle model, K. Sagarik and P. Asawakun 219 (1997) 173

Energy transfer processes
The unusual effect of reagent vibrational excitation on the rates of endothermic and exothermic elementary combustion reactions, A. Lifshitz and H. Teitelbaum 219 (1997) 243

Intramolecular dynamics
Molecular dynamics simulations of a potassium ion and an iodide ion in liquid ammonia, A. Tongraar, S. Hannongbua and B.M. Rode 219 (1997) 279

Non-linear responses (including optical)
Enhanced nonlinear optical properties and thermal stability of donor–acceptor substituted oligothiophenes, F. Steybe, F. Effenberger, S. Beckmann, P. Krämer, C. Glania and R. Wortmann 219 (1997) 317
Two-photon absorption in non-centrosymmetric dyes, S. Delysse, P. Raimond and J.-M. Nunzi 219 (1997) 341

Reactions (including dissociation)

-gas phase
The unusual effect of reagent vibrational excitation on the rates of endothermic and exothermic elementary combustion reactions, A. Lifshitz and H. Teitelbaum 219 (1997) 243

Tunnelling
Tunneling splitting in vibrational spectra of non-rigid molecules. I. Perturbative instanton approach, V.A. Benderskii, E.V. Vetoshkin, S.Yu. Grebenshchikov, L. von Laue and H.P. Trommsdorff 219 (1997) 119
Tunneling splitting in vibrational spectra of non-rigid molecules. II. Excited states, V.A. Benderskii, E.V. Vetoshkin, L. von Laue and H.P. Trommsdorff 219 (1997) 143

Electron transfer
Double exchange in tetrameric tetrahedral clusters with two-electron transfer: magnetic properties, V.P. Coropceanu, F.G. Paladi, S.I. Boldyrev and V.J. Gamurar 219 (1997) 1

Isotopic effects
A photoabsorption, photodissociation and photoelectron spectroscopy study of C_2H_4 and C_2D_4, D.M.P. Holland, D.A. Shaw, M.A. Hayes, L.G. Shpinkova, E.E. Rennie, L. Karlsson, P. Baltzer and B. Wannberg 219 (1997) 91

Surface effects and catalysis
"Free" nuclear density propagation in two dimensions. The coupled-channel density matrix method and its application to inelastic molecule–surface scattering, L. Pesce and P. Saalfrank 219 (1997) 43